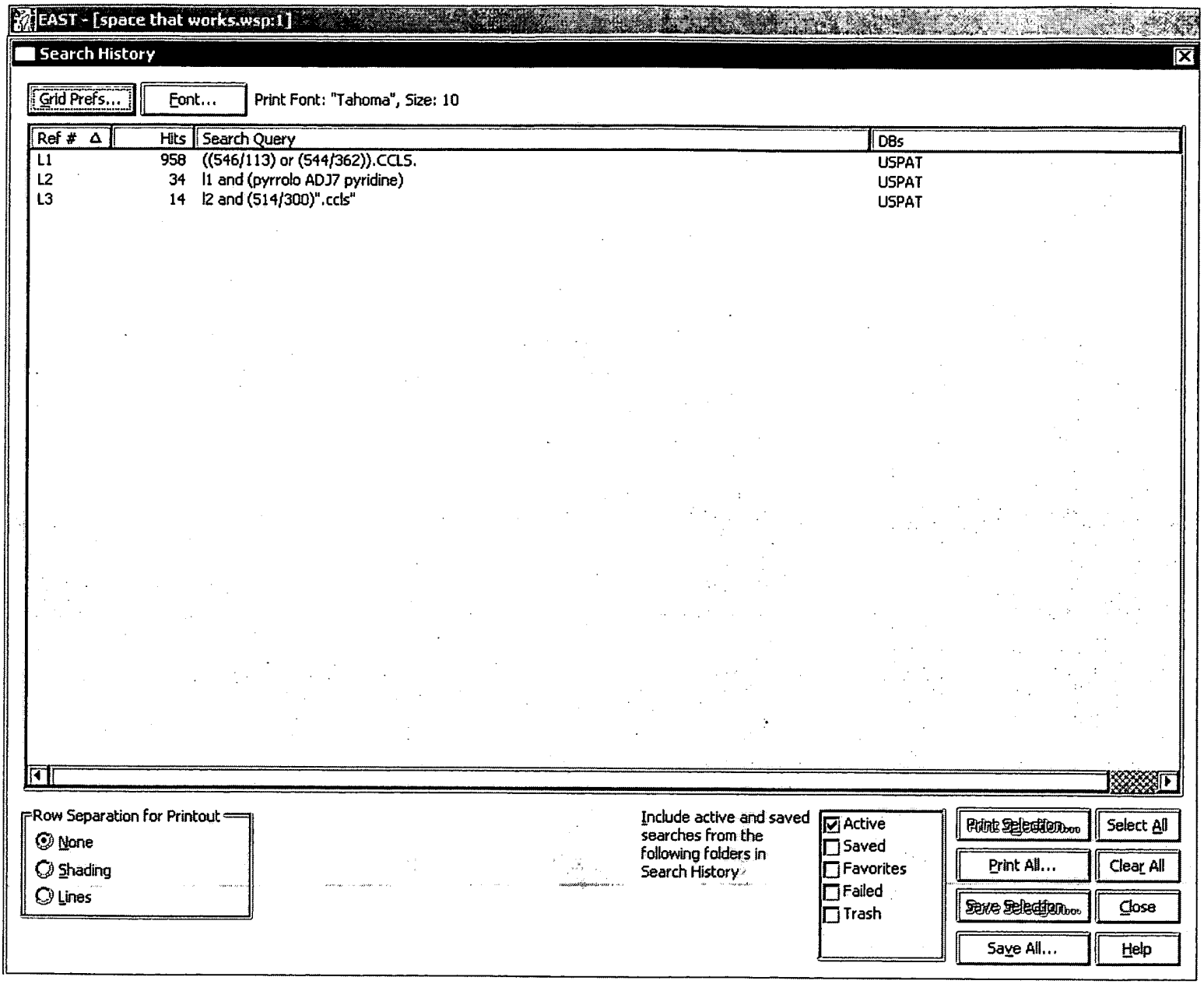
Inventor Information for 10/524361

Inventor Name	City	State/Country
NIELSEN, PETER AADAL	LUND	SWEDEN
BRIMERT, THOMAS	LUND	SWEDEN
KRISTOFFERSSON, ANNA	LUND	SWEDEN
LINNANEN, TERO	LUND	SWEDEN
SJO, PETER	LUND	SWEDEN

To go back use Back button on your browser toolbar.

Back to PALM | ASSIGNMENT | OASIS | Home page

10/524,361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L2 34 l1 and (pyrrolo ADJ7 pyridine) USPAT
L3 14 l2 and (514/300)".ccls" USPAT
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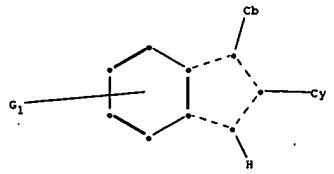
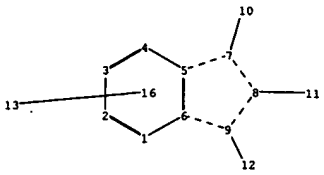
C:\Program Files\Stnexp\Queries\rkc361.str





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ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
7-10 8-11 9-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 8-11
exact bonds :
7-10 9-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:H,Cl,Br,F,I,CH3,Et,n-Pr,n-Bu,MeO,EtO,n-PrO,n-BuO,CN

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 16:Atom
Generic attributes :

10:
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Type of Ring System : Monocyclic
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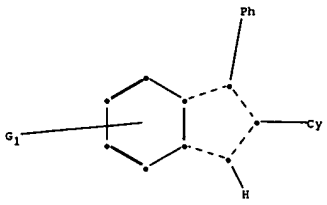
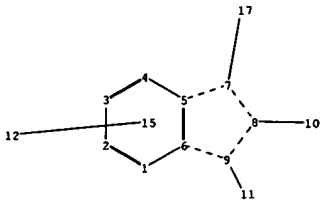
Type of Ring System : Monocyclic

C:\Program Files\Stnexp\Queries\rkc361b.str





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10 11 12 17
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
7-17 8-10 9-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 8-10
exact bonds :
7-17 9-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:H,Cl,Br,F,I,CH3,Et,n-Pr,n-Bu,MeO,EtO,n-PrO,n-BuO,CN

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS
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Generic attributes :

10:
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic

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L14           8 L13

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L14  ANSWER 1 OF 8  CAPLUS  COPYRIGHT 2007 ACS on STN
AN   2005:1103779  CAPLUS
DN   143:387011
TI   Preparation of azaindoles as inhibitors of JAK and other protein kinases
IN   Salituro, Francesco; Farmer, Luc; Bethiel, Randy; Harrington, Edmund;
     Green, Jeremy; Court, John; Come, Jon; Lauffer, David; Aronov, Alex;
     Binch, Hayley; Boyall, Dean; Charrier, Jean-Damien; Everitt, Simon;
     Fraysse, Damien; Mortimore, Michael; Pierard, Francoise; Robinson, Daniel
PA   Vertex Pharmaceuticals Incorporated, USA; et al.
SO   PCT Int. Appl., 432 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
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            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM,
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                                          US 2004-625599P     P  20041105
                                          WO 2005-US10846     W  20050330
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     EP 1730146           A1    20061213    EP 2005-756052           20050330
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            HR, LV, MK, YU
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OS   MARPAT 143:387011
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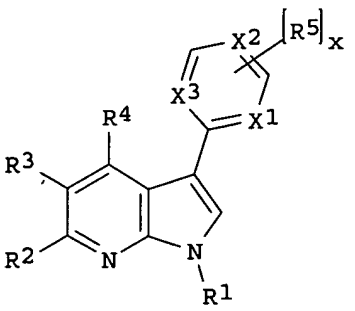

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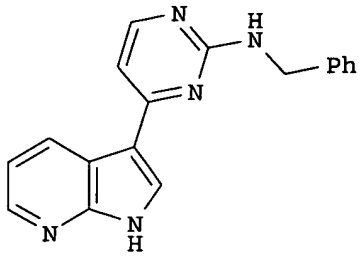


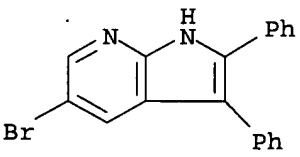
II

AB The title compds. I [R1 = TR', Si(R')3; R2-R4 = halo, CN, NO2, etc.; X1-X3 = N, CH (wherein the hydrogen atom of CH is optionally replaced by R5); x = 1-4; R5 = halo, CN, NO2, etc.; T = a bond, alkylidene, etc.; R' = H, alkyl, (hetero)cyclyl, etc.; with provisos] which are inhibitors of protein kinases, were prepared E.g., a multi-step synthesis of II, starting with 7-azaindole, was given. The compds. I were tested against JAK2, JAK3, ROCK and Aurora kinases (data given). The invention also provides pharmaceutical compns. comprising the compds. I and methods of using the compns. in the treatment of various disorders.

IT 664990-53-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azaindoles as inhibitors of JAK and other protein kinases)

RN 664990-53-8 CAPLUS

CN 1H-Pyrrolo[2,3-b]pyridine, 5-bromo-2,3-diphenyl- (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:162687 CAPLUS

DN 140:217627

TI Preparation of substituted pyrrolopyridines as Itk kinase inhibitors

IN Aadal Nielsen, Peter; Brimert, Thomas; Kristoffersson, Anna; Linnanen, Tero; Sjoe, Peter

PA Astrazeneca AB, Swed.

SO PCT Int. Appl., 74 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

	PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
PI	WO 2004016609	A1	20040226	WO 2003-SE1272		20030813
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	EP 1539757	A1	20050615	EP 2003-788209		20030813
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				WO 2003-SE1272	W	20030813
	US 2005261331	A1	20051124	US 2005-524626		20050210
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				WO 2003-SE1272	W	20030813

PATENT FAMILY INFORMATION:

FAN 2004:162688

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PI	WO 2004016610	A1	20040226	WO 2003-SE1275		20030813
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OS MARPAT 140:217627

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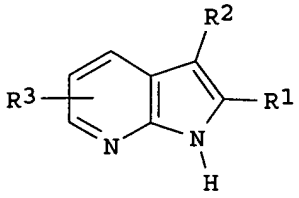


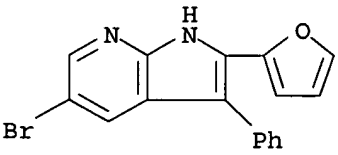
I

AB The title compds. [I; R1 = (un)substituted Ph, 5-6 membered aromatic heterocyclyl containing 1-3 heteroatoms selected from O, S and N; R2 = (un)substituted Ph, 5-6 membered aromatic heterocyclyl containing 1-3 heteroatoms selected from O, S and N; R3 = H, halo, alkyl, alkoxy, CN] and their salts, useful for treating or reducing the risk of a human disease or condition in which inhibition of Itk kinase activity is beneficial (such as asthma and allergic rhinitis), were prepared Thus, reacting 2-(4-methoxyphenyl)-1-phenylethanone with 5-bromo-2-hydrazinopyridine at 230° afforded 58% 5-bromo-3-(4-methoxyphenyl)-2-phenyl-1H-pyrrolo[2,3-b]pyridine. The exemplified compds. I showed IC50 of < 25 μM against Itk kinase. The pharmaceutical composition comprising the compound I is claimed.

IT 664990-48-1P 664990-53-8P 664990-54-9P
664990-58-3P 664990-63-0P 664990-64-1P
664990-65-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pyrrolopyridines as Itk kinase inhibitors)

RN 664990-48-1 CAPLUS

CN 1H-Pyrrolo[2,3-b]pyridine, 5-bromo-2-(2-furanyl)-3-phenyl- (9CI) (CA INDEX NAME)



RN 664990-53-8 CAPLUS

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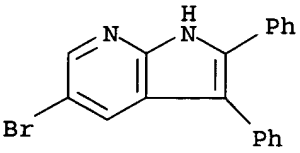

RN 664990-54-9 CAPLUS
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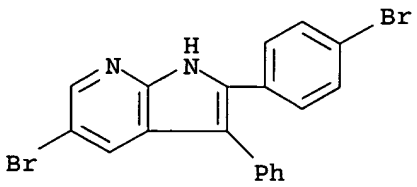

RN 664990-58-3 CAPLUS
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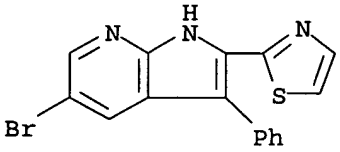
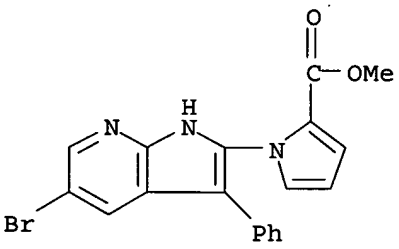


RN 664990-63-0 CAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 1-(5-bromo-3-phenyl-1H-pyrrolo[2,3-b]pyridin-2-yl)-, methyl ester (9CI) (CA INDEX NAME)



RN 664990-64-1 CAPLUS
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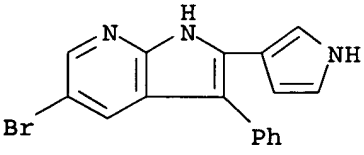
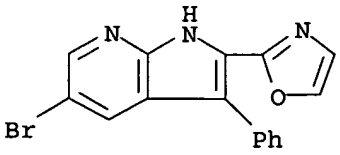
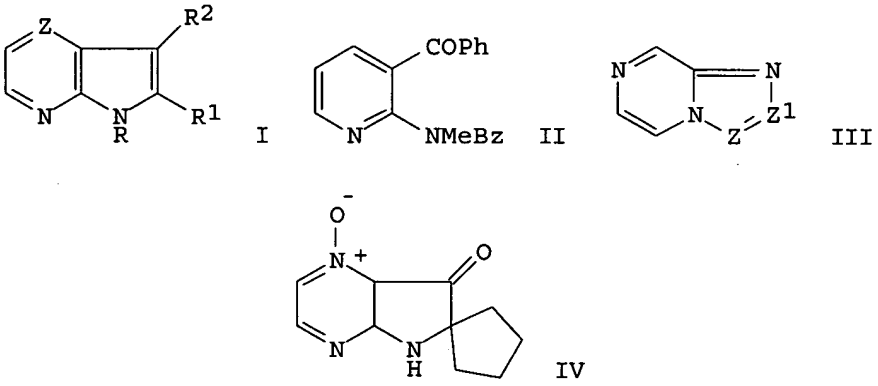


RN 664990-65-2 CAPLUS
CN 1H-Pyrrolo[2,3-b]pyridine, 5-bromo-2-(2-oxazolyl)-3-phenyl- (9CI) (CA INDEX NAME)



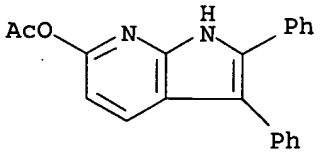
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1980:532395 CAPLUS
DN 93:132395
TI Ring opening or rearrangement versus N-oxidation in the action of peracids upon pyrrolo[2,3-b]pyridines, pyrrolo[2,3-b]pyrazines, and triazolo[1,5-a-]- and triazolo[4,3-a]pyrazine. Some chemical and spectroscopic properties of the triazolopyrazines and their N-oxides
AU Hardy, Christopher R.; Parrick, John
CS Sch. Chem., Brunel Univ., Uxbridge, UB3 3PH, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1980), (2), 506-11
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
OS CASREACT 93:132395
GI

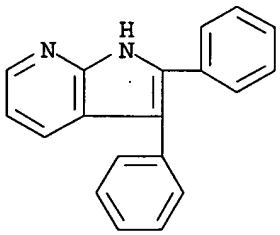


AB Peracid oxidation of the title compds. occurred by a variety of reaction pathways. E.g., the pyrrolopyridine and -pyrazines I (Z = CH, R = Me, R1 = R2 = Ph; Z = N, R = H, R1 = Ph, R2 = Me, resp.) ring-opened to give II and PhCONHCONH2, resp. In contrast, oxidation of the triazoles III (Z = N, Z1 = C; Z = C, Z1 = N, resp.) gave the resp. 7-oxides. The pyrrolopyrazine I [Z = N, R = Ac, R1R2 = (CH2)4] underwent rearrangement and N-oxidation to give the spiro compound IV. Some chemical and spectral properties of the triazolopyrazines and their N-oxides are reported.
IT 23616-69-5 74803-15-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylation of)

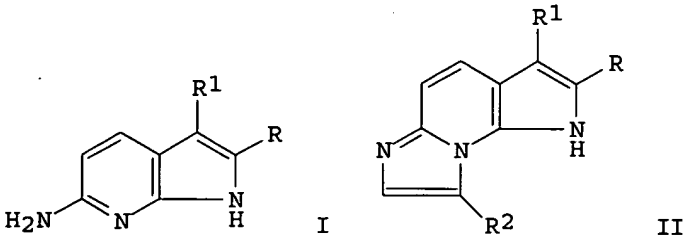
RN 23616-69-5 CAPLUS
CN 1H-Pyrrolo[2,3-b]pyridin-6-ol, 2,3-diphenyl-, acetate (ester) (8CI, 9CI) (CA INDEX NAME)



RN 74803-15-9 CAPLUS
CN 1H-Pyrrolo[2,3-b]pyridine, 2,3-diphenyl- (6CI, 9CI) (CA INDEX NAME)



L14 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1977:439361 CAPLUS
DN 87:39361
TI Synthesis and reactions of the 1H-imidazo[1,2-a]pyrrolo[3,2-e]pyridine system
AU Bancroft, Keith C. C.; Ward, Terence J.; Brown, Kevan
CS Sch. Chem., Leicester Polytech., Leicester, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1977), (5), 465-7
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
OS CASREACT 87:39361
GI



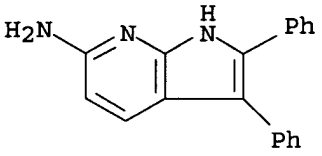
AB 6-Amino-1H-pyrrolo[2,3-b]pyridines with α-halocarbonyl compds. gave

1H-imidazo[1,2-a]pyrrolo[3,2-e]pyridines. E.g., I (R = Me, R1 = Me, H) with BrCH2CHO under reflux in aqueous EtOH in the presence of NaHCO3 gave 88 and 52% II (R = Me, R1 = Me, H, R2 = H, resp.). The imidazopyrrolopyridines underwent bromination, acetylation, and Mannich reactions at the 3-position; when the 3-position was blocked 8-substitution occurred. E.g., bromination of II (R = Me, R1 = Me, H, R2 = H) in CHCl3 gave 20 and 48% II (R = R1 = Me, R2 = Br; R = Me, R1 = Br, R2 = H, resp.).

IT 55463-74-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with halocarbonyl compds.)

RN 55463-74-6 CAPLUS

CN 1H-Pyrrolo[2,3-b]pyridin-6-amine, 2,3-diphenyl- (9CI) (CA INDEX NAME)



L14 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1975:4147 CAPLUS

DN 82:4147

TI Application of the Bischler reaction to the preparation of pyrrolopyridines and the novel dipyrrolopyridine system

AU Bancroft, Keith C. C.; Ward, Terence J.; Brown, Kevan

CS Sch. Chem., City Leicester Polytech., Leicester, UK

SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1974), (15), 1852-8
CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

LA English

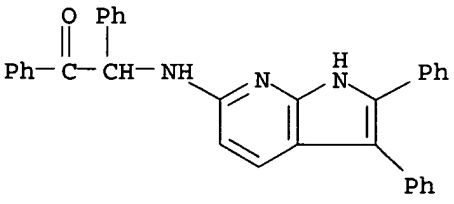
GI For diagram(s), see printed CA Issue.

AB The Bischler reaction of α-hydroxy ketones and 2,6-diaminopyridine gave 6-amino-1H-pyrrolo[2,3-b]pyridines and the 1,7-dihydrodipyrrolo[2,3-b:3',2'-e]pyridine system with various alkyl and aryl substituents. 2,6-Diphenyl-1,7-dihydrodipyrrolo[2,3-b:3',2'-e]-pyridine (I) underwent 3,5-disubstitution by electrophiles.

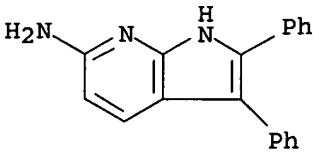
IT 55463-76-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 55463-76-8 CAPLUS

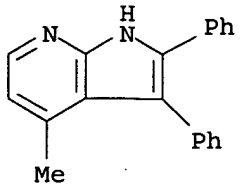
CN Ethanone, 2-[(2,3-diphenyl-1H-pyrrolo[2,3-b]pyridin-6-yl)amino]-1,2-diphenyl- (9CI) (CA INDEX NAME)



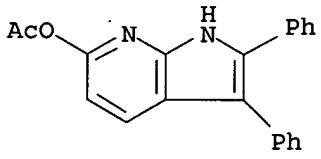
IT 55463-74-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzoine)
RN 55463-74-6 CAPLUS
CN 1H-Pyrrolo[2,3-b]pyridin-6-amine, 2,3-diphenyl- (9CI) (CA INDEX NAME)



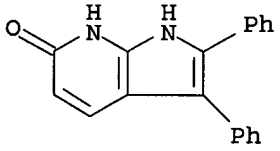
L14 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1969:449810 CAPLUS
DN 71:49810
TI Syntheses and properties of 1H-pyrrolo[2,3-b] pyridines
AU Herbert, R.; Wibberley, D. G.
CS Sch. Pharm., Sunderland Polytech., Sunderland, UK
SO Journal of the Chemical Society [Section] C: Organic (1969), (11), 1505-14
CODEN: JSOOAX; ISSN: 0022-4952
DT Journal
LA English
OS CASREACT 71:49810
GI For diagram(s), see printed CA Issue.
AB Five different routes for the preparation of 1H-pyrrolo[2,3-b]pyridines (I) were investigated. A number of 2-, 3-, and 4-alkyl and -aryl substituted derivs. were prepared by two of these methods which involved modifications of Madelung- and Fischer-syntheses of indoles. I undergo nitration, nitrosation, bromination, iodination, and reaction with Mannich bases predominantly at the 3-position although one example of nitration at the 2-position was also found. Bis[3-(1H-pyrrolo[2,3-b]-pyridyl)]methanes are formed by reaction with aldehydes, and treatment of 2-phenyl-1H-pyrrolo[2,3-b]pyridine with nitrosobenzene yields 2-phenyl-3-phenylimino-3H-pyrrolo[2,3-b]pyridine. A further example of a derivative of this isomeric 3H-system is 3-diazo-2-phenyl-3H-pyrrolo[2,3-b]pyridine which is formed from the corresponding amine by basification of the diazonium salt. 1-Substituted Grignard derivs. yield 3-iodo-compds. on treatment with H2O2 but only 1-acyl derivs. with acyl chlorides. Treatment of 2-phenyl-1H-pyrrolo[2,3-b]pyridine with CHCl3 and alkali caused ring-expansion to a 1,8-naphthyridine. A number of unexpected products were isolated both in the syntheses of the 1H-pyrrolo[2,3-b]pyridines and in their reactions with electrophiles. Ir, N.M.R., and mass spectra were used to establish all structures.
IT 23612-72-8P 23616-69-5P 23616-70-8P
23616-71-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23612-72-8 CAPLUS
CN 1H-Pyrrolo[2,3-b]pyridine, 4-methyl-2,3-diphenyl- (8CI) (CA INDEX NAME)



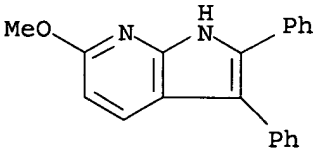
RN 23616-69-5 CAPLUS
CN 1H-Pyrrolo[2,3-b]pyridin-6-ol, 2,3-diphenyl-, acetate (ester) (8CI, 9CI) (CA INDEX NAME)



RN 23616-70-8 CAPLUS
CN 1H-Pyrrolo[2,3-b]pyridin-6-ol, 2,3-diphenyl- (8CI) (CA INDEX NAME)



RN 23616-71-9 CAPLUS
CN 1H-Pyrrolo[2,3-b]pyridine, 6-methoxy-2,3-diphenyl- (8CI) (CA INDEX NAME)



L14 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1959:94804 CAPLUS
DN 53:94804
OREF 53:17126h-i,17127a-i,17128a
TI 7-Azaindole. V. Investigations of alternative syntheses of the ring system
AU Okuda, Shigenobu; Robison, Michael M.
CS Amherst Coll., Amherst, MA
SO Journal of the American Chemical Society (1959), 81, 740-3
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
OS CASREACT 53:94804
AB cf. C.A. 51, 13860g. 5,6,7,8-Tetrahydro-9H-pyrido[2,3-b]indole (I) and

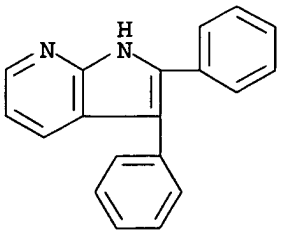
2,3-diphenyl-7-azaindole (II) were prepared by Fischer cyclizations of the corresponding pyridylhydrazones with polyphosphoric acid (III), though the method failed for a number of simpler pyridylhydrazones. 2-Aminopyridine-3-acetic acid (IV), obtained in low yield by a sequence from 3-(cyanomethyl)pyridine N-oxide (V), was also converted to 7-azaoxindole (VI). Cyclohexanone (VII) (4.90 g.) added to 5.45 g. 2-pyridylhydrazine (VIIa), the resulting white powder triturated with H2O, and recrystd. from cyclohexane and aqueous EtOH yielded the 2-pyridylhydrazone (VIII) of VII, m. 92-2.5° with sintering at about 85° (all m.ps. are corrected). VIII (5.68 g.) and 18 g. III heated gradually (to about 160°) to initiate the vigorous reaction, the mixture cooled, dissolved in 100 cc. H2O, washed with Et2O, neutralized with NH4OH, the product sublimed at 110°/0.2 mm. and recrystd. from aqueous EtOH yielded 2.75 g. I, m. 155-6°. I (0.001 mol), 0.1 g. 5% Pd-C, and 5 cc. Dowtherm refluxed 2 h., cooled, added to 5 cc. C6H6, filtered, extracted with warm dilute HCl, and the extract basified with NH4OH precipitated 0.14 g. 9H-pyrido[2,3-b]indole, m. 210.5-11° (C6H6). PhCH(OH)Bz (IX) (1.96 g.) in 1 cc. glacial AcOH and 1.09 g. VIIa kept 2.5 h. at room temperature and the solid deposit triturated with dilute NH4OH and EtOH gave 1.4 g. 2-pyridylhydrazone (X) of IX, b0.3 160°, m. 110°. X (1.8 g.) and 8 g. III heated 1 h. at 110-20°, cooled, stirred with 20 cc. warm H2O, and extracted with C6H6, the aqueous layer and solid basified with NH4OH, the organic layer extracted with Et2O, and the extract worked up yielded 0.21 g. II, m. 292.5-3.5° (BuOH) (sublimed at 230°/0.1 mm.). Desyl chloride (2.31 g.) in 10 cc. 95% EtOH refluxed with 0.94 g. 2-aminopyridine, the EtOH distilled, the mixture heated 1 h. at 130-40° and 5 min. to 190°, cooled, treated with H2O and NH4OH, and diluted with Me2CO precipitated 1.14 g. 2,3-diphenylimidazo[1,2-a]pyridine, plates, m. 151-1.5° (MeCN). NaCN (30 g.) in 45 cc. hot H2O treated with stirring with 250 cc. 95% EtOH and then dropwise with stirring during 40 min. with 20 g. 3-(chloromethyl)pyridine-HCl in 50 cc. 95% EtOH and 20 cc. H2O, refluxed 1 h. with stirring, evaporated in vacuo, the residue extracted with Et2O, and the extract worked up yielded 76.5-82.5% 3-(cyanomethyl)pyridine (XI), b7 126°, n20D 1.5279. XI (11.0 g.), 55 cc. glacial AcOH, and 15 cc. 30% H2O2 heated 12 h. on the steam bath, cooled to room temperature, treated again with 10 cc. H2O2, heated 8 h., diluted with 70 cc. H2O, evaporated in vacuo, treated with H2O and evaporated again repeatedly, extracted with CHCl3, and the extract worked up gave 10.8 g. V, m. 135.5-6.5° (CHCl3-C6H6). V (10.0 g.) added to 100 cc. POCl3, warmed slowly with vigorous shaking, refluxed 2 h., evaporated in vacuo, the brown sirupy residue poured onto 160 g. ice, filtered, and the residue recrystd. from Et2O-petr. ether gave 2.55 g. 2-Cl derivative (XII) of XI, m. 85-6° (Et2O-petr. ether). The strongly acidic, aqueous filtrate extracted with CHCl3, the extract worked up, and the residue chromatographed on 80 g. Al2O3 yielded 1.44 g. XII and 0.91 g. 2-chloro-5-(cyanomethyl)pyridine (XIII), m. 48-50°; the intermediate fractions combined with the recrystn. mother liquors from the XII and rechromatographed on 50 g. Al2O3 yielded an addnl. 0.52 g. XII, 0.65 g. XIII, and 0.7 g. XII-XIII mixture; the crude XIII recrystd. from Et2O-petr. ether gave pure XIII, m. 51-2°. The aqueous layer from the CHCl3 extns. adjusted to pH 4 with NH4OH and extracted with CHCl3, basified with NH4OH and again extracted, and the extract worked up gave only intractable tars; the aqueous layer evaporated to dryness in vacuo, the residue extracted with

boiling Me2CO, and the extract evaporated gave 0.78 g. 3-hydroxy-5-(cyanomethyl)pyridine (XIV), m. 180-1° (C6H6-Me2CO), orange-red with FeCl3. XII (0.5 g.) and 20 cc. concentrated HCl refluxed 5.5 h. and evaporated to dryness in vacuo, the residue triturated with H2O, dissolved in dilute aqueous NaHCO3, filtered, and repptd. with acid gave 0.43 g. 2-chloro-3-pyridineacetic acid (XV), m. 203-4° (C6H6). XII (265 mg.) and 614 mg. KMnO4 in 20 cc. H2O heated 20 min. on the steam bath, filtered, saturated with CO2, evaporated in vacuo, the residue dissolved in H2O, filtered, repptd. with acid, and recrystd. from H2O yielded 232 mg. 2-chloronicotinic acid, m. 192-3° (decomposition). XIII oxidized similarly yielded 50% 6-chloronicotinic acid, m. 198-9°. XIV (0.35 g.) and 10 cc. concentrated HCl refluxed 5 h., evaporated in vacuo, the residue dissolved in 10 cc. H2O, treated with saturated aqueous Cu(OAc)2, the precipitate filterd off, washed with a small amount cold H2O, suspended in 40 cc. MeOH, treated with H2S, filtered, and evaporated, and the residue recrystd. from MeOH-EtAc gave 0.31 g. 3-hydroxy-5-pyridineacetic acid (XVI), m. 197° (decomposition). XVI (0.2 g.) heated 15 min. under N at 230° and the residue sublimed at 135/0.05 mm. gave 0.11 g. 3-hydroxy-5-methylpyridine, m. 138.5° (C6H6); picrate m. 189-90°. XII (0.5 g.), 0.1 g. CuSO4.5H2O, and 15 cc. concentrated NH4OH heated 42 h. in a sealed tube at 135 ± 10°, filtered, evaporated in vacuo, and the residue treated with 5 cc. cold H2O gave 105 mg. IV, m. 219-21.5° (decomposition), crystallizing with 0.5 mol H2O. The aqueous filtrate from the crude IV treated with H2S, filtered, evaporated in vacuo, the residue extracted with hot absolute EtOH, the extract evaporated, the residue dissolved in 5 cc. absolute EtOH, the solution diluted with 30 cc. Me2CO, filtered, concentrated to 1/3 the original volume, and the pale orange deposit (0.11 g.) recrystd. from absolute EtOH-C6H6 and H2O gave 23 mg. 2-hydroxy-3-pyridineacetic acid (XVII), m. 240-1° (decomposition). XV (0.16 g.) in 10 cc. 5% aqueous NaOH heated 4.5 h. in an autoclave at 200°, filtered, acidified with concentrated HCl, evaporated, the residue extracted with boiling MeOH, and the extract worked up gave 95 mg. XVII, m. 240-1° (decomposition), red color with FeCl3. IV (0.1 g.) heated 10 min. under N at 225° and the residue sublimed at 170°/10 mm. yielded 56 mg. VI, m. 175°.

IT 74803-15-9P, 1H-Pyrrolo[2,3-b]pyridine, 2,3-diphenyl-
RL: PREP (Preparation)
(preparation of)

RN 74803-15-9 CAPLUS

CN 1H-Pyrrolo[2,3-b]pyridine, 2,3-diphenyl- (6CI, 9CI) (CA INDEX NAME)



L14 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1947:25604 CAPLUS
DN 41:25604
OREF 41:5126f-i,5127a-i,5128a-f
TI Derivatives of 2,6-diaminopyridine
AU Bernstein, Jack; Stearns, Barbara; Shaw, Elliott; Lott, W. A.
CS Squibb Inst. for Med. Research, New Brunswick, NJ
SO Journal of the American Chemical Society (1947), 69, 1151-8
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
OS CASREACT 41:25604
AB Since 2,6-diaminopyridine (I) showed an appreciable antiparasitic activity when tested against Plasmodium lophurae in ducklings, various derivs. of I have been prepared to determine if further substitution in the mol. would increase the antiparasitic activity of the parent compound I (66 g.) in 300 cc. dioxane, treated dropwise with 23.5 g. AcCl in 50 cc. dioxane (0.5 h.) at 25-30° and stirred 2 addnl. hrs., gives 40% of the 2-Ac derivative (II), m. 156-7°; 2-butyryl derivative m. 152-3°, 25%; 2-salicyloyl derivative (prepared from o-AcOC6H4COCl and purified by precipitation from dilute HCl with dilute NaOH) m. 178-9°, 44%; 2-[phenyl(acetoxy)acetyl] derivative (as HCl salt with 1 mol. H2O) m. 151-3°, 23%. N,N'-Bis(6-amino-2-pyridyl)adipamide m. 228-9°, 72%; N,N'-bis(6-amino-2-pyridyl)sebacamide m. 152-5°, 55%. 1,3-Bis(6-amino-2-pyridyl)urea does not melt, 71%. (CH2CO)2O (30 g.) in 200 cc. dioxane, treated slowly with 33 g. I in 200 cc. dioxane and heated 3 h. on the steam bath, gives 57% N-(6-amino-2-pyridyl)succinamic acid, m. 174-5° (decomposition). I (46 g.) and 222 cc. AcCH2CO2Et, heated 15 min. at 160° and the product in EtOH treated with alc. HCl, give 40% 2,6-bis(acetylacetamido)pyridine-HCl, m. 195-8°; the filtrate yields 10% of the 2-acetylacetamido derivative, m. 146-7°. I (22 g.) and 22.6 g. NCCH2CO2Et, heated 2 h. at 165°, give 85% 2-amino-6-cyanoacetamidopyridine, m. 152-3°. 2-Acetamido-6-carbethoxyacetamidopyridine m. 150-1.5°, 41%. I (282 g.) and 290 g. HOCH2CO2H, fused 15 h. at 120° under reduced pressure, give 35% 2,6-bis(glycolylamino)pyridine, m. 220-1°. I (33 g.) in 200 cc. absolute EtOH containing 6.9 g. Na and 43 g. Et2NCH2CO2Et, refluxed 2 h., give 55% 2,6-bis(diethylaminoacetamido)pyridine, m. 109.5-10.5°. I (22 g.) and 27 g. AcNHCOCl, ground in a mortar and 35 cc. C5H5N added, give 19% 2,6-bis(acetamidoacetamido)pyridine, m. 260-1°. MeC(:NH)NH2.HCl (24.6 g.) in 100 cc. absolute EtOH, added to 22 g. I in 150 cc. absolute EtOH, stirred 3 h., and allowed to stand overnight at room temperature, give 38% N-(6-amino-2-pyridyl)acetamidine-HCl, m. 246-7° (decomposition). I (396 g.) in 8 l. H2O, treated dropwise with 195 g. ClCO2Et (3 h.), gives 76% 2-amino-6-carbethoxyaminopyridine (III), m. 109-12°. I (33 g.) in 500 cc. H2O, 200 cc. N HCl, and 300 g. ice, treated dropwise with 33 g. ClCO2Et, stirred 2 h., 200 cc. N HCl added, and the mixture allowed to stand overnight at 10°, gives 55% 2,6-bis(carbethoxyamino)pyridine, m. 132.5-3.5°, and 12 g. III. III (21.6 g.) in 120 cc. 3 N EtOH-NH3, heated 12 h. at 110°, gives 75% 2-amino-6-ureidopyridine, m. 175-6° (decomposition). I (48 g.) and 48 g. CO(NH2)2, heated 36 h. at 130°, give 49% 2,6-diureidopyridine, does not melt below 300° (purified by extraction with 300 cc. 3% HCl and crystallization of the residue from H2O). I (12 g.) in 1500 cc. C6H6, treated dropwise with 17.9 g. p-EtOC6H4NCO in 75 cc. C6H6, gives 86% 2-(p-ethoxyphenylureido)-6-aminopyridine, m. 168-9°; 2-(2-nitro-4-methoxyphenylureido)-6-aminopyridine m. 208-10°, 73%; reduction over Pt oxide gives 50% of the corresponding 2-(2-amino-4-methylphenylureido) derivative, m. 182-4°.

I (154 g.) and 200 g. of the HCl salt of I, heated 12 h. at 190°, give 60% bis(6-amino-2-pyridyl)amine, m. 172-3° (the HCl salt does not melt). 2,6-Dibromopyridine (IV) (38 g.) and 160 cc. 25% aqueous MeNH2, heated 8 h. at 190°, give 59% 2,6-bis(methylamino)pyridine, m. 70-1°; this results in 20% yield from 27.6 g. 2-amino-6-bromopyridine (V) and 110 cc. 25% aqueous MeNH2 on heating 30 h. at 190°. V (80 g.) and 200 cc. EtNH2, heated 36 h. at 170-80°, give 81% 2-amino-6-(diethylamino)pyridine (VI), b4.5 122-3°, m. 34-5° (HCl salt, m. 143-4°). IV (45 g.) and 27.8 g. Et2NH in 100 cc. absolute EtOH, heated 8 h. at 170-80°, give 85% 2-bromo-6-(diethylamino)pyridine (VII), b4 97-9°; VII does not react with NH4OH (d. 0.9) at 170-80° (8 h.); 11 g. VII and 35 cc. 5 N EtOH-NH3, heated 25 h. at 170°, also did not react; 18.8 g. VII in 100 cc. NH4OH (d. 0.9) containing 1 g. CuSO4.5H2O, heated 30 h. at 140-5°, gives 44% VI. IV (35.6 g.) and 100 cc. Et2NH containing 4 cc. 25% CuSO4.5H2O, heated 30 h. at 160°, give 76% 2,6-bis(diethylamino)pyridine, b3 120-2° (HCl salt, m. 120-2°). 2-Amino-6-(3-diethylaminopropylamino)pyridine-HCl m. 65-75°, 53%; 2-acetamido-6-(4-diethylamino-1-methylbutylamino)pyridine m. 106-8° (51%). 2-Acetamido-6-(3-keto-1-methylbutylideneamino)-pyridine, 2,6-AcNHC5H3N(N:CMeCH2Ac), m. 146-7.5°, 40%. 2-Acetamido-6-(2,5-dimethyl-1-pyrryl)pyridine m. 147.5-8.5°, 54%. 2-Methoxy-6,9-dichloroacridine (11.2 g.) in 50 g. PhOH, warmed on the steam bath, treated with 11 g. I, and heated 3 h., gives 61% 2-methoxy-6-chloro-9-(6-amino-2-pyridylamino)acridine, yellow, m. 232-3°. II (30.2 g.), added in small portions to 100 cc. HNO3 (d. 1.5) at -5° to -2° and stirred an addnl. 30 min., gives 65% of the Ac derivative, decompose violently at 193°, of 2-nitramino-6-aminopyridine (VIII), darkens at 240-50° (hydrolysis by refluxing 1 h. with N NaOH); reduction of 15.4 g. VIII in 300 cc. 10% NaOH at 0-2° with 31 g. Zn gives 69% 2-hydrazino-6-aminopyridine, pale yellow, m. 93-4°; warmed 2 h. on the steam bath with AcCH2CO2Et (N atmospheric), there results 44%
1- (6-amino-2-pyridyl)-3-methyl-5-pyrazolone, m. 188-9.5°. 3-Methylpyridine (80 g.), 160 g. PhNMe2, and 144 g. NaNH2, heated 10 h. at 130-50° and 6 h. at 170-200°, give 4% 2,6-diamino-3-methylpyridine, m. 149-50°. 2,6-Dihydroxy-4-methylpyridine (9 g.) and 30 g. PBr3, heated 4.5 h. at 180°, give 36% 2,6-dibromo-4-methylpyridine, m. 74-5°; heated with NH4OH (d. 0.9) 27 h. at 195°, there results 71% 2,6-diamino-4-methylpyridine, m. 87-8°, which on sublimation m. 109-11° but reverts to the lower m.p. on standing. 2,6-Diamino-3-iodopyridine (23.5 g.) in 25 cc. AcOH and 35 cc. Ac2O, heated 1 h. on the steam bath, gives 33% of the di-Ac derivative, m. 210-11°. I (38 g.) in 550 cc. H2O, treated with 93 g. iodine and 93 g. KI in 150 cc. H2O, the mixture stirred 8 h., and allowed to stand overnight at room temperature, gives 36% 2,6-diamino-3,5-diiodopyridine-HCl, m. 160-5°; the free base m. 209-10°.
3-Methoxypyridine (IX) (15.8 g.) in 100 cc. concentrated H2SO4, treated dropwise (with cooling) with 25 cc. HNO3 (d. 1.6) and warmed 6 h. on the steam bath, gives 12.2 g. 3-methoxy-2,6-dinitropyridine (X), m. 114-15°. IX (57 g.), added to 130 cc. concentrated H2SO4 at 5°, the mixture treated with 70 cc. HNO3 (d. 1.6), and heated 1 h. on the steam bath, yields 38 g. 2-nitro-3-methoxypyridine (XI), m. 73-5°; 5 g. XI in 15 cc. concentrated H2SO4, treated with 4 cc. HNO3 (d. 1.6), gives 4.4 g. X. Catalytic reduction (Pt oxide) of 16.8 g. X in 500 cc. AcOH and 250 cc. Ac2O at room temperature (4 h.) gives 60% 3-methoxy-2,6-diacetamidopyridine, m. 173.5-4.5°. 2,3,6-Triaminopyridine-2HCl in 200 cc. H2O and 25 g. Ac2 in 200 cc. H2O, boiled 4 min., yield 98% 2,3-dimethyl-6-aminopyrido[2,3]pyrazine, m.

227-8°; 6-aminopyrido[2,3]pyrazine m. 267°, 62%.
2,3,6-Triaminopyridine oxalate (80 g.) in 150 cc. (CO2Et)2, heated 90 min. at 185°, gives 68% 2,3-dihydroxy-6-aminopyrido[2,3]pyrazine, does not m. below 300°. Addition of 23.8 g. 2,6-diacetamido-3-nitropyridine to 100 g. SnCl2.2H2O in 150 cc. concentrated HCl gives 26% 2-methyl-5-amino-1-imidazo[b]pyridine-HCl; neither the base nor the salt melts. I (55 g.) and 194 g. KCNS in 1 l. 95% AcOH, treated dropwise at -5° to -10° with 26 cc. Br, give 24% 2,5-diaminopyrido[2,3-d]thiazole (XII), m. 138-9°; II likewise gives the 5-Ac derivative of XII, m. 184-5°. I (66 g.) in 2 l. AcOH, treated with 460 g. KCNS in 100 cc. H2O and then at 0-3° with 64 cc. Br, with stirring 1 h. at room temperature, yields 22% 2,6-diaminopyrido[2,3-d,6,5-d']bisthiazole, does
not melt below 300°. I (25 g.), 29 g. I.HCl, and 42 g. benzoin, heated 1 h. at 185°, yield 89% 2,3-diphenyl-6-amino-1-pyrrolo[2,3-b]pyridine, m. 234.5-5.5°. 2-Amino-6-(3-keto-1-methylbutylideneamino)pyridine (16 g.) in 100 cc. 85% H3PO4, warmed 1 h. on the steam bath, gives 84% 2,4-dimethyl-7-amino-1,8-naphthyridine, m. 216-18°; this results in 85% yield from 5 g. I and 5 cc. CH2Ac2 in 25 cc. 85% H3PO4 on warming 30 min. on the steam bath.
2,7-Dihydrazino-4-methyl-1,8-naphthyridine-2HCl-2H2O (23 g.) and 18 g. AcCH2CO2Et in 200 cc. 50% EtOH, heated 5 min. at 70°, give 84% 2,7-bis(3-methyl-5-keto-1-pyrazolyl)-4-methyl-1,8-naphthyridine, m. 260-2°. The most active of these compds. (II, XII, and the di-Ac derivative of I) are only 1/3 as active as quinine as antiparasitic agents for Plasmodium lophurae in ducklings.

IT 55463-74-6P, 1H-Pyrrolo[2,3-b]pyridine, 6-amino-2,3-diphenyl-
RL: PREP (Preparation)
(preparation of)

RN 55463-74-6 CAPLUS

CN 1H-Pyrrolo[2,3-b]pyridin-6-amine, 2,3-diphenyl- (9CI) (CA INDEX NAME)